

Lyapunov Exponent for Pure and Random Fibonacci Chains

M. T. Velinho and I. R. Pimentel[†]

Department of Physics and CFMC, University of Lisbon, Lisboa 1649, Portugal

Abstract

We study the Lyapunov exponent for electron and phonon excitations, in pure and random Fibonacci quasicrystal chains, using an exact real space renormalization group method, which allows the calculation of the Lyapunov exponent as a function of the energy. It is shown that the Lyapunov exponent on a pure Fibonacci chain has a self-similar structure, characterized by a scaling index that is independent of the energy for the electron excitations, "diagonal" or "off-diagonal" quasiperiodic, but is a function of the energy for the phonon excitations. This scaling behavior implies the vanishing of the Lyapunov exponent for the states on the spectrum, and hence the absence of localization on the Fibonacci chain, for the various excitations considered. It is also shown that disordered Fibonacci chains, with random tiling that introduces phason flips at certain sites on the chain, exhibit the same Lyapunov exponent as the pure Fibonacci chain, and hence this type of disorder is irrelevant, either in the

case of electron or phonon excitations.

PACS: 71.23.Ft, 71.23-k, 63.50.+x

1 Introduction

The experimental discovery of quasicrystals,¹ and also the building of artificial multilayer structures by molecular beam epitaxy,² have considerably stimulated the theoretical study of quasiperiodic systems.³⁻⁵ Quasicrystals have a deterministic aperiodicity that characterizes them as intermediate structures between periodic crystals and disordered materials, therefore being expected to display new behavior. There has been in particular, great discussion on the nature of the energy spectrum and eigenstates of electron and phonon excitations on quasicrystals. It is questioned whether the spectrum is absolutely continuous, pointlike or singular continuous, or correspondingly, if the states are extended, localized or critical.

The Fibonacci chain is the simplest quasicrystal, a one-dimensional system where the site or bond variables take one of the two values A and B , and are arranged in a Fibonacci sequence. The Fibonacci chain can be constructed recursively by successive applications of a substitution rule, $A \rightarrow AB$ and $B \rightarrow A$, or alternatively, by successive applications of a concatenation rule, $S_i = S_{i-1} \otimes S_{i-2}$, S_i being the Fibonacci sequence at iteration i . The quasiperiodicity of the Fibonacci chain is characterized by the golden mean $\tau = (1 + \sqrt{5})/2$, which gives the ratio of the number of A and B units. Tight-binding electron and phonon excitations have been studied on a Fibonacci

chain, using mainly transfer-matrix^{6–12} and real space renormalization group techniques.^{13–15} It has been found that the energy spectrum for these excitations is a Cantor set with zero Lebesgue measure, this result having in addition been proven¹⁶ for the case of electronic excitations on a site Fibonacci chain. The spectra of the periodic approximants to the Fibonacci chain exhibit self-similarity in the band structure, with a scaling index that for the electronic excitations is independent of the energy, while for the phonon excitations it is a function of the energy.⁹ The integrated density of states for the various excitations presents rich scaling behavior, with indices varying from the edge to the center of the bands.^{10–12,14} The characterization of the eigenstates on a Fibonacci chain is a more difficult task, and it has usually been restricted to a few special energies on the spectrum, for which the states are found to be self-similar or chaotic. More generally, it has been found evidence for the states being neither extended nor localized in the usual sense.^{10–12}

The localization properties of the states can be studied through the calculation of the Lyapunov exponent γ , which characterizes the evolution of a wavefunction along the chain.^{17–19} The Lyapunov exponent is zero for an extended or critical state, but is positive for a localized state representing then the inverse of the localization length. Delyon and Petritis²⁰ have proved that the Lyapunov exponent for a class of binary quasiperiodic tight-binding chains, vanishes on the spectrum, which rules out the presence of localized states. The Fibonacci sequence does not however belong to this class of chains, and the characterization of the states in that case remains under discussion. A study

on localization lengths of tight-binding electrons on a pure Fibonacci chain has been presented by Capaz *et al.*,²¹ that found no evidence for localization of the states.

Real systems have in general some disorder. Random quasicrystals, in the sense of a random tiling, have been considered²² to explain the properties of quasicrystalline alloys. It is well known that disorder has pronounced effects on the transport properties of periodic systems, specially in one-dimension where all the states turn to localized whatever the amount of disorder. A striking property of quasicrystals is that they exhibit extremely high resistivities, which decrease with the amount of defects.²³ The effects of some types of disorder on the electronic spectra and wavefunctions of Fibonacci chains have been considered.^{24–26}

In this work we study the Lyapunov exponent for electron and phonon excitations in pure and random Fibonacci quasicrystal chains. We consider electrons in a tight-binding model, with "diagonal"-site and "off-diagonal"-bond Fibonacci ordering, and phonons on a lattice with bond Fibonacci ordering. The disorder introduced is random tiling imposed on the substitution or concatenation rules for construction of the Fibonacci chains. We use a real space renormalization group method, which allows the calculation of a wavefunction along the chain, for any given energy, and therefore enables the determination of its Lyapunov exponent. This method provides a simple and very efficient way of numerically calculating the Lyapunov exponent as a function of the energy, for large Fibonacci chains. The method has great similarities, but also important differences, as will be discussed, with that used by Capaz *et al.*²¹ The

method is based on decimation, which is here applied either to substitution¹⁴ or concatenation,²⁵ and implemented in the presence of disorder.

In order to calculate an eigenstate, one needs to specify an energy on the spectrum. Since the spectrum of a Fibonacci chain is a Cantor set with zero Lebesgue measure, the probability of numerically specifying an energy on the spectrum is essentially zero. Hence any chosen energy will almost certainly correspond to a gap, and the calculated Lyapunov exponents are then associated to gap states. It is shown that the Lyapunov exponent for the gap states of the various excitations has a fractal structure, and we study its scaling properties. From these properties we obtain information on the Lyapunov exponent for the states on the spectrum of the Fibonacci chain, and therefore on the localization properties of the excitations. We study the Lyapunov exponent for both, tight-binding electrons and phonons, remarking that the Goldstone symmetry present in the latter and absent in the former, may lead to important differences in the scaling properties of the two systems.

The outline of the paper is as follows. In Sec. II we describe the tight-binding electron and phonon systems that are studied, and present the renormalization method used to calculate the Lyapunov exponent. In Sec. III we present the Lyapunov exponent for the various excitations on a pure Fibonacci chain, study its scaling properties and discuss localization, and finally consider the effects of disorder on the Lyapunov exponent. In Sec. IV we present our conclusions.

2 Renormalization approach

The dynamics of tight-binding electron and phonon excitations on a Fibonacci quasicrystal chain, can be described by the generic equation

$$(\varepsilon_n - E)\Psi_n = V_{n-1}\Psi_{n-1} + V_n\Psi_{n+1}. \quad (1)$$

For the electrons, Ψ_n denotes the amplitude of the wavefunction at site n , corresponding to energy E , ε_n is a site energy, and V_n is the hopping amplitude between site n and $n + 1$. For phonons, Ψ_n represents the displacement from the equilibrium position of the atom at site n , $E = m\omega^2$, ω being the phonon frequency and m the atom mass, $\varepsilon_n = V_{n-1} + V_n$, and V_n is the spring constant connecting sites n and $n + 1$. This latter model describes equally well spin waves on an Heisenberg ferromagnet at zero temperature, replacing the spring constants by exchange constants, and $m\omega^2$ by the spin wave frequency ω . We note the Goldstone symmetry present in the phonon system, which imposes a correlation between the site ε_n and the coupling V_n parameters, that is not present in the electron system.

The various Fibonacci quasicrystal models are defined as follows. For electrons, the "diagonal" model is obtained from (1) by setting, $V_n = 1$ and $\varepsilon_n = \varepsilon_A$ or ε_B , according to the Fibonacci sequence, and the "off-diagonal" model is obtained from (1) by setting, $\varepsilon_n = 0$ and $V_n = V_A$ or V_B , according to the Fibonacci sequence. The model for phonons is obtained from (1) with the couplings $V_n = V_A$ or V_B , arranged in the Fibonacci sequence.

The disordered Fibonacci chains are built by introducing random tiling in the substitution rule for construction,

$$\begin{aligned}
B &\rightarrow A, \\
A &\rightarrow AB, \text{ probability } p, \\
A &\rightarrow BA, \text{ probability } 1 - p,
\end{aligned} \tag{2}$$

in each iteration i , starting with B , the two possibilities corresponding respectively to direct and inverse substitution, or they are built by introducing random tiling in the concatenation rule for construction,

$$\begin{aligned}
S_i &= S_{i-1} \otimes S_{i-2}, \text{ probability } p, \\
S_i &= S_{i-2} \otimes S_{i-1}, \text{ probability } 1 - p,
\end{aligned} \tag{3}$$

starting with $S_0 = B$ and $S_1 = A$, the two possibilities corresponding respectively to direct and inverse concatenation. Random tiling on substitution or concatenation generates, at each iteration, an identical set of disordered Fibonacci chains, though through a different sequence of preceeding chains (e.g. $A \rightarrow AB \rightarrow ABA \rightarrow ABABA$, by substitution, vs, $A \rightarrow BA \rightarrow AAB \rightarrow ABABA$, by concatenation).

The method that we use to calculate the Lyapunov exponent is based on the fact that the wavefunction Ψ_n at the Fibonacci sites $n = n(i) = F_{i+1}$, given by $F_{i+1} = F_i + F_{i-1}$ with $F_1 = F_0 = 1$, can be easily obtained via a real-space renormalization group transformation, which consists in eliminating

appropriated sites on the chain, so that a chain similar to the original one is obtained, with a rescaled length and renormalized parameters. Under successive decimations one carries the system through larger length scales separating the sites. For the Fibonacci chain it is possible to deduce an exact renormalization transformation for the parameters ε_n and V_n , the rescaling factor, under which the system is self-similar, being equal to τ . After i iterations, the renormalization transformation takes, for example, V_A to $V_A^{(i)}$, which represents the renormalized interaction between two sites that are a distance τ^i apart, measured in units of the original lattice spacing. The Fibonacci sites $n(i)$ become the first neighbours of the end site $n = 0$, at each iteration i . Now, writing (1) as a recursion relation for the wavefunction, and fixing the "free-end" boundary condition $V_{-1} = 0$, one gets, $\Psi_1 = [(\varepsilon_0 - E)/V_0] \Psi_0$. The wavefunction Ψ_n at the consecutive Fibonacci sites $n(i)$, can therefore be obtained in terms of the parameters under successive renormalization iterations i , through

$$\Psi_{n(i)} = \left[\left(\varepsilon_0^{(i)} - E \right) / V_0^{(i)} \right] \Psi_0, \quad (4)$$

fixing Ψ_0 (e.g. $\Psi_0 = 1$). The Lyapunov exponent γ is then calculated from the wavefunction (4), given that

$$|\Psi_n| \sim e^{\gamma x_n}, \quad (n \rightarrow \infty), \quad (5)$$

and $x_n = \tau^i$ for $n = n(i)$. In the work of Capaz *et al.*²¹ the localization of the wavefunction Ψ is studied following the behavior of the coupling V under successive renormalizations, and not through the evolution of the wavefunction (4),

which also involves the parameter ε . Although the behaviour of Ψ is mainly determined by V , the complete expression should be used. Furthermore, in that work a small imaginary part η is added to the energy E , which produces an artificial decay of the coupling V , that alters the actual evolution of the wavefunction, and consequently interferes in the study of localization and evaluation of the Lyapunov exponent.

Now we present the decimation techniques used to obtain the renormalization transformation of the parameters ε_0 and V_0 , for chains constructed by substitution or concatenation.

A. Substitution chains

The renormalization transformation of the parameters is obtained by eliminating sites in such a way as to reverse the substitution procedure in (2).¹⁴ In order to build the transformation one needs to consider an expanded parameter space, for the various excitations, where the bonds V_n assume two different values, V_A and V_B , arranged in a Fibonacci sequence, and the site energies ε_n may assume three different values, depending on the local environment of n , ε_α if $V_{n-1} = V_n = V_A$, ε_β if $V_{n-1} = V_A$ and $V_n = V_B$, ε_γ if $V_{n-1} = V_B$ and $V_n = V_A$. A choice of the initial parameters V_A , V_B , ε_α , ε_β , ε_γ , casts the problem into the model for electron excitations, "diagonal" ($V_A = V_B$, $\varepsilon_\alpha = \varepsilon_\gamma \neq \varepsilon_\beta$) or "off-diagonal" ($V_A \neq V_B$, $\varepsilon_\alpha = \varepsilon_\beta = \varepsilon_\gamma$), or phonon excitations ($V_A \neq V_B$, $\varepsilon_\alpha = 2V_A$, $\varepsilon_\beta = \varepsilon_\gamma = V_A + V_B$). The reversal of rule (2) is achieved through the elimination of β - sites, corresponding to direct substitution, or γ -sites,

corresponding to inverse substitution. The resulting renormalization equations

are:

i) direct substitution,

$$\begin{aligned}
\varepsilon_\alpha^{(i+1)} &= \varepsilon_\gamma^{(i)} - \left(V_A^{(i)2} + V_B^{(i)2} \right) / \left(\varepsilon_\beta^{(i)} - E \right), \\
\varepsilon_\beta^{(i+1)} &= \varepsilon_\gamma^{(i)} - V_B^{(i)2} / \left(\varepsilon_\beta^{(i)} - E \right), \\
\varepsilon_\gamma^{(i+1)} &= \varepsilon_\alpha^{(i)} - V_A^{(i)2} / \left(\varepsilon_\beta^{(i)} - E \right), \\
V_A^{(i+1)} &= V_A^{(i)} V_B^{(i)} / \left(\varepsilon_\beta^{(i)} - E \right), \quad V_B^{(i+1)} = V_A^{(i)},
\end{aligned} \tag{6}$$

and for the end site $n = 0$,

$$\varepsilon_0^{(i+1)} = \varepsilon_0^{(i)} - V_A^{(i)2} / \left(\varepsilon_\beta^{(i)} - E \right), \quad V_0^{(i+1)} = V_A^{(i+1)}, \tag{7}$$

ii) inverse substitution,

$$\begin{aligned}
\varepsilon_\alpha^{(i+1)} &= \varepsilon_\beta^{(i)} - \left(V_A^{(i)2} + V_B^{(i)2} \right) / \left(\varepsilon_\gamma^{(i)} - E \right), \\
\varepsilon_\beta^{(i+1)} &= \varepsilon_\alpha^{(i)} - V_A^{(i)2} / \left(\varepsilon_\gamma^{(i)} - E \right), \\
\varepsilon_\gamma^{(i+1)} &= \varepsilon_\beta^{(i)} - V_B^{(i)2} / \left(\varepsilon_\gamma^{(i)} - E \right), \\
V_A^{(i+1)} &= V_A^{(i)} V_B^{(i)} / \left(\varepsilon_\gamma^{(i)} - E \right), \quad V_B^{(i+1)} = V_A^{(i)},
\end{aligned} \tag{8}$$

and for the end site $n = 0$,

$$\begin{aligned}
\varepsilon_0^{(i+1)} &= \varepsilon_0^{(i)} - V_B^{(i)2} / \left(\varepsilon_\gamma^{(i)} - E \right), \quad V_0^{(i+1)} = V_A^{(i+1)}, \quad \text{if } V_0^{(i)} = V_B^{(i)}, \\
\varepsilon_0^{(i+1)} &= \varepsilon_0^{(i)}, \quad V_0^{(i+1)} = V_B^{(i+1)}, \quad \text{if } V_0^{(i)} = V_A^{(i)}.
\end{aligned} \tag{9}$$

B. Concatenation chains

The renormalization transformation of the parameters is obtained by eliminating the central site, after having performed concatenation, so as to reverse the concatenation procedure (3).²⁵ This leads to the following renormalization equations, which are different for bond Fibonacci ordering, i.e. "off-diagonal" electrons and phonons, or site Fibonacci ordering, i.e. "diagonal" electrons.

For the bond problem:

i) direct concatenation,

$$\begin{aligned}\varepsilon_0^{(i+1)} &= \varepsilon_0^{(i)} - V_0^{(i)2} / \left(\varepsilon_{cd}^{(i+1)} - E \right), \\ \varepsilon_{F_{i+1}}^{(i+1)} &= \varepsilon_{F_{i-1}}^{(i-1)} - V_0^{(i-1)2} / \left(\varepsilon_{cd}^{(i+1)} - E \right), \\ V_0^{(i+1)} &= V_0^{(i)} V_0^{(i-1)} / \left(\varepsilon_{cd}^{(i+1)} - E \right),\end{aligned}\tag{10}$$

with, $\varepsilon_{cd}^{(i+1)} = \varepsilon_{F_i}^{(i)} + \varepsilon_0^{(i-1)}$,

ii) inverse concatenation,

$$\begin{aligned}\varepsilon_0^{(i+1)} &= \varepsilon_0^{(i-1)} - V_0^{(i-1)2} / \left(\varepsilon_{ci}^{(i+1)} - E \right), \\ \varepsilon_{F_{i+1}}^{(i+1)} &= \varepsilon_{F_i}^{(i)} - V_0^{(i)2} / \left(\varepsilon_{ci}^{(i+1)} - E \right), \\ V_0^{(i+1)} &= V_0^{(i)} V_0^{(i-1)} / \left(\varepsilon_{ci}^{(i+1)} - E \right),\end{aligned}\tag{11}$$

with, $\varepsilon_{ci}^{(i+1)} = \varepsilon_{F_{i-1}}^{(i-1)} + \varepsilon_0^{(i)}$, and the initial values, $V_0^{(0)} = V_B$, $V_0^{(1)} = V_A$, $\varepsilon_0^{(0)} = \varepsilon_1^{(0)} = \varepsilon_0^{(1)} = \varepsilon_1^{(1)}$, for "off-diagonal" electrons, and $\varepsilon_0^{(0)} = \varepsilon_1^{(0)} = V_0^{(0)} = V_B$, $\varepsilon_0^{(1)} = \varepsilon_1^{(1)} = V_0^{(1)} = V_A$, for phonons.

For the site problem:

i) direct concatenation,

$$\begin{aligned}
\varepsilon_0^{(i+1)} &= \varepsilon_0^{(i)} - V_0^{(i)2} / \left[\left(\varepsilon_{F_i}^{(i)} - E \right) - T^2 / \left(\varepsilon_0^{(i-1)} - E \right) \right], \\
\varepsilon_{F_{i+1}}^{(i+1)} &= \varepsilon_{F_{i-1}}^{(i-1)} - V_0^{(i-1)2} / \left[\left(\varepsilon_0^{(i-1)} - E \right) - T^2 / \left(\varepsilon_{F_i}^{(i)} - E \right) \right], \\
V^{(i+1)} &= TV_0^{(i)} V_0^{(i-1)} / \left[\left(\varepsilon_0^{(i-1)} - E \right) \left(\varepsilon_{F_i}^{(i)} - E \right) - T^2 \right],
\end{aligned} \tag{12}$$

ii) direct concatenation,

$$\begin{aligned}
\varepsilon_0^{(i+1)} &= \varepsilon_0^{(i-1)} - V_0^{(i-1)2} / \left[\left(\varepsilon_{F_{i-1}}^{(i-1)} - E \right) - T^2 / \left(\varepsilon_0^{(i)} - E \right) \right], \\
\varepsilon_{F_{i+1}}^{(i+1)} &= \varepsilon_{F_i}^{(i)} - V_0^{(i)2} / \left[\left(\varepsilon_0^{(i)} - E \right) - T^2 / \left(\varepsilon_{F_{i-1}}^{(i-1)} - E \right) \right], \\
V^{(i+1)} &= TV_0^{(i)} V_0^{(i-1)} / \left[\left(\varepsilon_0^{(i)} - E \right) \left(\varepsilon_{F_{i-1}}^{(i-1)} - E \right) - T^2 \right],
\end{aligned} \tag{13}$$

with the initial values, $V_0^{(2)} = T$, $\varepsilon_0^{(3)} = \varepsilon_2^{(3)} = \varepsilon_A - T^2 / (\varepsilon_B - E)$, $V_0^{(3)} = T^2 / (\varepsilon_B - E)$, and in i) $\varepsilon_0^{(2)} = \varepsilon_A$, $\varepsilon_1^{(2)} = \varepsilon_B$, while in ii) $\varepsilon_0^{(2)} = \varepsilon_B$, $\varepsilon_1^{(2)} = \varepsilon_A$.

Considering the general case of a random Fibonacci chain, for a given probability of disorder p , we start with a specific disordered configuration, generated by (2) or (3), respectively for substitution or concatenation chains, and then iterate (6) – (9), (10) – (11) or (12) – (13), depending on the system studied, according to that configuration, in order to obtain the successive values for $V_0^{(i)}$ and $\varepsilon_0^{(i)}$. This allows us to calculate the wavefunction Ψ_n , provided by (4), at the successive Fibonacci sites, for a given energy E . For each probability p , we average the obtained wavefunction for E over many different disorder configurations. It is important to remark that when dealing with random chains, one

should first calculate the wavefunction for a specific disordered configuration and then average over configurations, instead of averaging the parameters over disorder at each step of the renormalization and then calculate the wavefunction with the averaged parameters. This latter procedure²⁵ will wash out important correlations in the system, and leads to different results depending on how the average is performed. The first procedure describes the physics more accurately.

3 Lyapunov Exponent for Fibonacci Chains

We now present the results concerning the Lyapunov exponent, calculated as a function of the energy, for the tight-binding electron, "diagonal" and "off-diagonal", and phonon excitations on the pure and random Fibonacci chains. We consider first the case of pure chains, for which we study the scaling properties of the Lyapunov exponent and their implications for the localization of states on the spectrum, and analyse afterwards the effects of disorder, of the kind of random tiling, on the Lyapunov exponent.

As mentioned above, the wavefunctions that we numerically calculate correspond to gap states. Figure 1 shows the typical behavior of a wavefunction Ψ_n , at any chosen energy E , either for the electron or the phonon excitations on a pure Fibonacci chain. One observes that the wavefunction first oscillates over a certain length, and then grows exponentially. This behavior has mixed characteristics of an extended (oscillating) state and a localized (exponential) state. The length over which a wavefunction oscillates is a "memory" length,¹⁰

in the sense that beyond this length it loses memory of its initial phase. The exponential growth of the wavefunction is characterized by the Lyapunov exponent, which measures the inverse of a "localization length". We find that the "memory" length ξ and the Lyapunov exponent γ are simply related, $\xi \approx 1/\gamma$. In figure 2 we present the Lyapunov exponent for the electron, "diagonal" and "off-diagonal", and phonon excitations on the pure Fibonacci chain, calculated as a function of the energy. The exponent exhibits a rather nontrivial dependence on the energy, which has a clear correspondence with the associated density of states obtained by Ashraff and Stinchcombe^{14,15} for the various cases, the finite values of the Lyapunov exponent corresponding to gap states, with the further a state is inside a gap the larger is its Lyapunov exponent. The Lyapunov exponent exhibits a fractal structure, i.e. under dilation the same structure is revealed in a smaller scale, as can be seen by comparing the Lyapunov plots in figure 2 with those in figure 3. This structure is observed even in the very low energy range of the magnetic excitations, where γ takes particularly small values, most probably due to the Goldstone symmetry.

The scaling behavior of the Lyapunov exponent is studied through the variation of the maximum exponent in a gap, γ_{\max} , versus the gap width, ΔE_g .²¹ We find that

$$\gamma_{\max} \sim (\Delta E_g)^\delta, \quad (14)$$

where the scaling index δ , is independent of the energy for the electron excitations, "diagonal" and "off-diagonal", as shown in figure 4, but depends on

the energy for the phonon excitations, as figure 5 reveals, and it is shown in figure 6. We also find that the scaling index for the electron excitations depends on the quasicrystal site ($\varepsilon_A, \varepsilon_B$) or bond (V_A, V_B) parameters, decreasing as the difference between the parameters increases, while the scaling index for the phonon excitations, varying with energy, also depends on the quasicrystal parameters (V_A, V_B). Our results for the electron excitations are in agreement with those obtained by Capaz et al.,²¹ though their scaling indices differ from ours, probably due to the fact that they have calculated the Lyapunov exponent from the behavior of the coupling V alone and not from the evolution of the wavefunction Ψ , in (4), and moreover have introduced an imaginary part in the energy which influences the Lyapunov exponent, as discussed earlier.

From the scaling expression (14), one obtains, for the various excitations, that $\gamma_{\max} \rightarrow 0$ when $\Delta E_g \rightarrow 0$, implying that the Lyapunov exponent for wavefunctions on the spectrum, vanishes. We therefore have that the electron, "diagonal" or "nondiagonal", and phonon excitations on a Fibonacci chain are nonlocalized.

Let us now study the effects of disorder on the Lyapunov exponent. Disorder has drastic effects on the wavefunctions of one-dimensional periodic systems, localizing all the states. Figure 7 illustrates this fact, showing the Lyapunov exponent for phonon excitations on a random periodic chain, with couplings V_A and V_B , as a function of the probability p of disorder, for various energies. One sees that the Lyapunov exponent increases with disorder, being also an increasing function of the energy.

For the random Fibonacci chains we considered disorder of the kind of random tiling, introduced in the substitution or concatenation rule for construction of the chains. The resulting disordered chains differ from the pure Fibonacci chain in having a varying number of phason flips, located at certain points on that chain. By a phason flip it is meant a local rearrangement of tiles on the quasiperiodic structure, corresponding to a switch of the site, ε_A and ε_B , or the bond, V_A and V_B , parameters.²⁶ Using the cyclic property of the trace one can see that all those random tiling chains have the same spectrum, for the electron and the phonon excitations, as the pure Fibonacci chain. In the work of López *et al.*,²⁵ on the effects of that kind of random tiling on the electronic excitations of a Fibonacci chain, it has however been found that the disorder affects the spectrum of the excitations. We think that this result is a consequence of the averaging of the parameters over disorder taken at each step of the renormalization in that work, which as already mentioned, loses important correlations in the system and introduces effects that depend on the averaging procedure used, corresponding in fact to different systems. On the other hand Naumis and Aragón,²⁶ considering electronic excitations, have also noted that phason flips located at certain points on the Fibonacci chain do not alter the spectrum of the excitations.

We calculated the Lyapunov exponent for the electron and phonon excitations on Fibonacci chains with random tiling, as a function of the probability of disorder, for different values of energy. The results obtained are illustrated in figure 8. We find that the disorder considered does not affect the Lyapunov

exponent either for the electron, "diagonal" or "off-diagonal", or the phonon excitations. The same result is obtained for disordered Fibonacci chains with random tiling either in the substitution or the concatenation rule for construction of chains. The irrelevance of disorder found for the Lyapunov exponent of excitations on a Fibonacci chain is surprising, knowing the drastic effects that disorder has on the excitations on periodic chains. However, it should be noted that random tiling introduces a kind of bounded disorder, which has also correlations, and therefore might not be sufficient to produce localization of states. Furthermore, in contrast to the general case, it has been reported that there exist particular random potentials in one dimension that allow for extended states, those being described by an iterative procedure of construction.^{27,28} Liu and Riklund²⁴ have found that other types of disorder, different from the one considered by us, produce localization of electronic excitations on a Fibonacci chain.

4 Conclusions

We have studied the Lyapunov exponent for tight-binding electron, "diagonal" and "off-diagonal", and phonon excitations in pure and random Fibonacci quasicrystal chains, using a real space renormalization group method. This method allows the calculation of a wavefunction along the chain, and the determination of the associated Lyapunov exponent, as a function of the energy, in a very efficient way for very long chains. We have found that the Lyapunov exponent

for the pure Fibonacci chain has a self-similar structure, being characterized by a scaling index that is independent of the energy for the electronic excitations, but depends on the energy for the phonon excitations. The scaling properties of the Lyapunov exponent, imply that it vanishes on the spectrum for the various excitations. We therefore have that the electronic and phonon excitations are nonlocalized on the Fibonacci chain . Considering random Fibonacci chains, we calculated the Lyapunov exponent as a function of the probability of disorder, and found that the disorder introduced, of the kind of random tiling, does not affect the Lyapunov exponent, which takes the same value as for the pure Fibonacci chain whatever the degree of disorder, either for the electron or for the phonon excitations. The random tiling considered generates in fact chains that are locally isomorphic to the pure Fibonacci chain, and therefore our results imply that locally isomorphic chains, besides having the same energy spectrum,²⁹ also have the same Lyapunov exponent, and hence their eigenstates have the same nature as the ones of the pure Fibonacci chain. We are now investigating the effects of random tiling on the Lyapunov exponent, of electron and phonon excitations, on other aperiodic chains, such as the Thue-Morse, the period-doubling, and binary non-Pisot sequences. Other types of disorder are also being considered on the Fibonacci chain, as well as on the other aperiodic chains mentioned, in order to understand the relevance/irrelevance of disorder on the Lyapunov exponent, and consequently on the localization properties of those systems. The results of this work will be reported elsewhere.

Acknowledgements

We would like to thank R. B. Stinchcombe and J. M. Luck for very helpful conversations.

References

[†]iveta@alf1.cii.fc.ul.pt

- ¹D. Shechtman, I. Blech, D. Gratias and J. W. Cahn, Phys. Rev. Lett. **53**, 1951 (1984).
- ²R. Merlin, K. Bajena, R. Clarke, F. Y. Juang, and P. K. Bhattacharya, Phys. Rev. Lett. **5**, 1768 (1985).
- ³P. J. Steinhardt and S. Ostlund, *The Physics of Quasicrystals* (World Scientific, Singapore, 1987).
- ⁴D. P. DiVicenzo and P. Steinhardt, *Quasicrystals: The State of the Art* (World Scientific, Singapore, 1991).
- ⁵C. Janot, *Quasicrystals - a primer*, 2nd. ed. (Clarendon Press, Oxford, 1994).
- ⁶M. Kohmoto, L. P. Kadanoff and C. Tang, Phys. Rev. Lett. **50**, 1870 (1983).
- ⁷S. Ostlund and R. Pandit, Phys. Rev. B **29**, 1394 (1984).
- ⁸M. Kohmoto and Y. Oono, Phys. Lett. **102A**, 145 (1984).
- ⁹M. Kohmoto and J. Banavar, Phys. Rev. B **34**, 563 (1986).
- ¹⁰J. M. Luck and D. Petritis, J. Stat. Phys. **42**, 289 (1986).
- ¹¹M. Kohmoto, B. Sutherland and C. Tang, Phys. Rev. B **35**, 1020 (1987).
- ¹²B. Sutherland, Phys. Rev. B **35**, 9529 (1987).
- ¹³Q. Niu and F. Nori, Phys. Rev. Lett. **57**, 2057 (1986).
- ¹⁴J. A. Ashraff and R. B. Stinchcombe, Phys. Rev. B **37**, 5723 (1988).
- ¹⁵J. A. Ashraff, D.Phil. Thesis, Oxford 1989.
- ¹⁶A. Süto, J. Stat. Phys. **56**, 525 (1989).
- ¹⁷K. Ishii, Supp. Progr. Theor. Phys. **53**, 77 (1973).

- ¹⁸J. M. Luck, *Systèmes Désordonnés Unidimensionnels* (Collection Aléa - Saclay, 1992).
- ¹⁹A. Crisanti, G. Paladin and A. Vulpiani, *Products of Random Matrices*, Vol. 104 of Springer Series in Solid-State Sciences (Springer, Berlin, 1993).
- ²⁰F. Delyon and D. Petritis, Commun. Math. Phys. **103**, 441 (1986).
- ²¹R. B. Capaz, B. Koiller and S. L. A. Queiroz, Phys. Rev. B **42**, 6402 (1990).
- ²²C. L. Henley, in Ref. 4, p. 429.
- ²³K. Kimura and S. Takeuchi, in Ref. 4, p.313.
- ²⁴Y. Liu and R. Riklund, Phys. Rev. B **35**, 6034 (1987).
- ²⁵J. C. López, G. Naumis and J. L. Aragón, Phys. Rev. B **48**, 12459 (1993).
- ²⁶G. G. Naumis and J. L. Aragón, Phys. Lett. A **244**, 133 (1998).
- ²⁷J. S. Denbigh and N. Rivier, J. Phys. C **12**, L107 (1979).
- ²⁸A. Crisanti, C. Falesia, A. Pasquarella, and A. Vulpiani, J. Phys.: Condens. Matter **1**, 9509 (1989).
- ²⁹F. Wijnands, J. Phys. A **22**, 3267 (1989).

Figure captions

FIG. 1. Inverse of the phonon wavefunction Ψ_n at the Fibonacci sites $n = F_{i+1}$, for energy $E = 0.4$, on a pure Fibonacci chain, and the associated Lyapunov exponent γ .

FIG. 2. Lyapunov exponent γ for: a) electronic "diagonal" ($\varepsilon_\alpha = -\varepsilon_\beta = \varepsilon_\gamma = 1$), b) electronic "off-diagonal" ($V_A = 1, V_B = 2$), and c) phonon ($V_A = 1, V_B = 2$) excitations on a pure Fibonacci chain.

FIG. 3. Self-similar structure of γ : a) electronic "diagonal" ($\varepsilon_\alpha = -\varepsilon_\beta = \varepsilon_\gamma = 1$), b) electronic "off-diagonal" ($V_A = 1, V_B = 2$), and c) phonon ($V_A = 1, V_B = 2$) excitations, to compare with FIG. 2.

FIG. 4. Maximum γ in a gap vs gap width ΔE_g , for: a) electronic "diagonal", (\blacktriangle) ($\varepsilon_\alpha = -\varepsilon_\beta = \varepsilon_\gamma = 1, \delta = 0.62$), (\blacksquare) ($\varepsilon_\alpha = -\varepsilon_\beta = \varepsilon_\gamma = 2, \delta = 0.47$); b) electronic "off-diagonal", (\bullet) ($V_A = 1, V_B = 2, \delta = 0.75$), (\blacklozenge) ($V_A = 3, V_B = 1, \delta = 0.53$), excitations on a pure Fibonacci chain.

FIG. 5. Maximum γ in a gap vs gap width ΔE_g , for phonon excitations ($V_A = 1, V_B = 2$), on a pure Fibonacci chain.

FIG. 6. Power-law exponent δ , of γ_{\max} vs ΔE_g , for phonon excitations: a) $V_A = 1, V_B = 2$, b) $V_A = 2, V_B = 1$, on a pure Fibonacci chain.

FIG. 7. Lyapunov exponent γ vs probability of disorder p , for phonon excitations, with energies: (\bullet) $E = 1.2$, (\blacklozenge) $E = 2.3$, (\blacktriangle) $E = 3.4$, on random periodic chains.

FIG. 8. Lyapunov exponent γ vs probability of disorder p , for various energies E , of: a) electronic "diagonal", (\bullet) $E = -1.9$, (\blacklozenge) $E = 0.15$, (\blacktriangle) $E = 1.1$; b) electronic "off-diagonal", (\bullet) $E = 0.5$, (\blacklozenge) $E = 1.5$, (\blacktriangle) $E = 2.05$, c) phonon, (\bullet) $E = 1.4$, (\blacklozenge) $E = 3.1$, (\blacktriangle) $E = 5.29$, excitations on random Fibonacci chains.

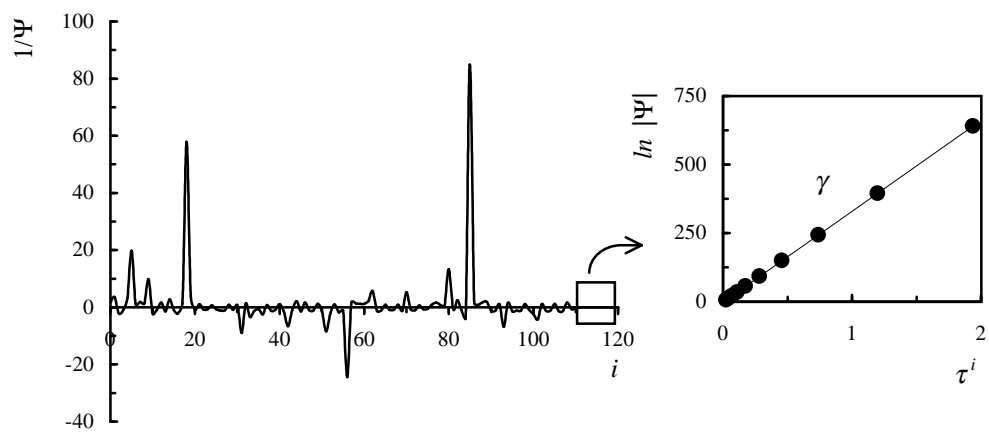
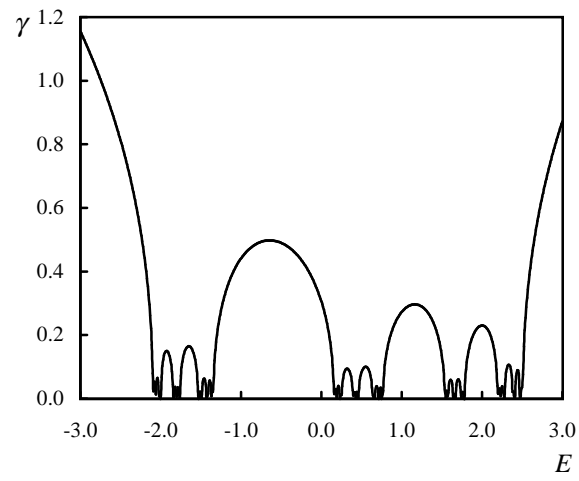
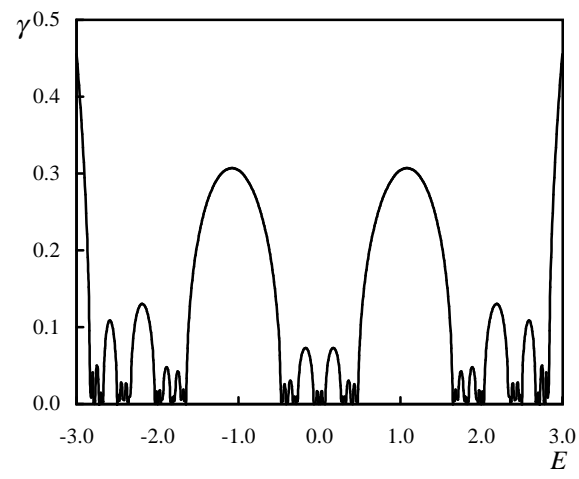


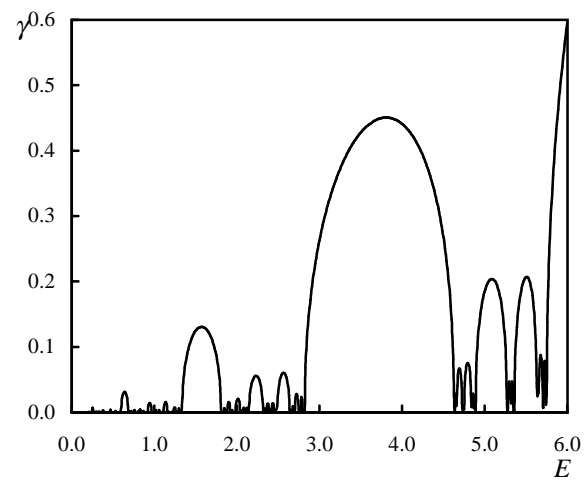
FIG. 1



(a)

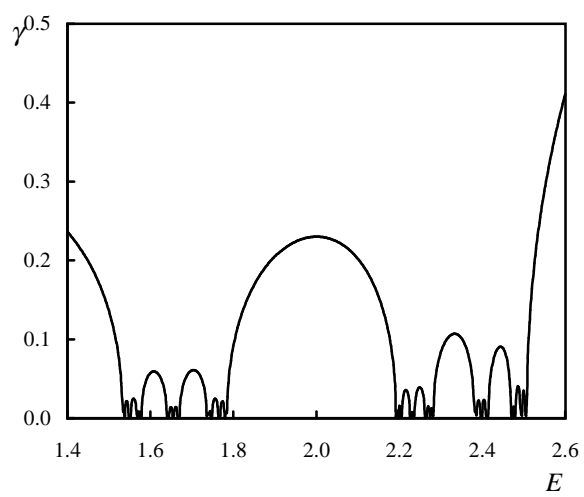


(b)

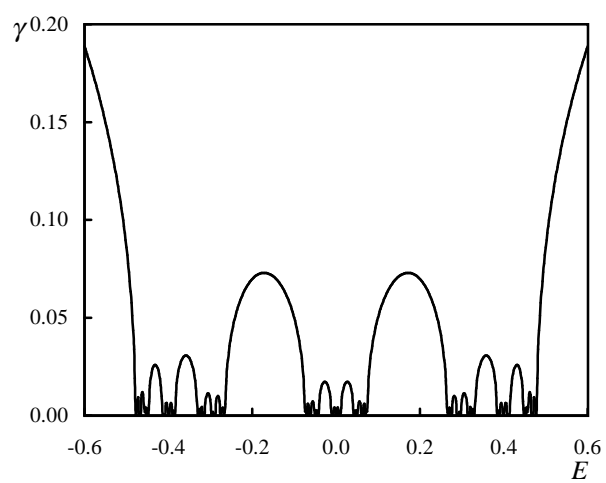


(c)

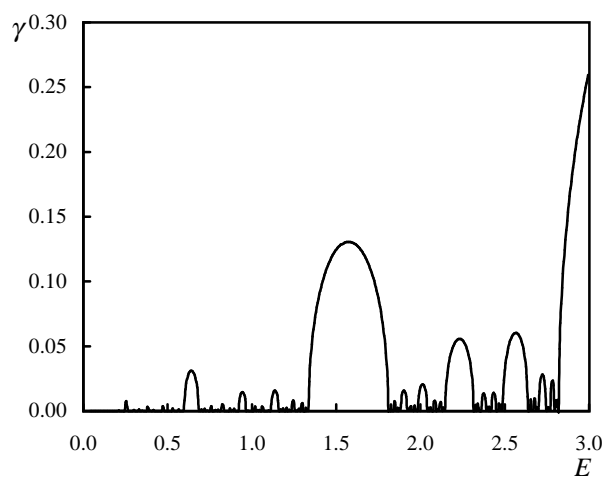
FIG. 2



(a)

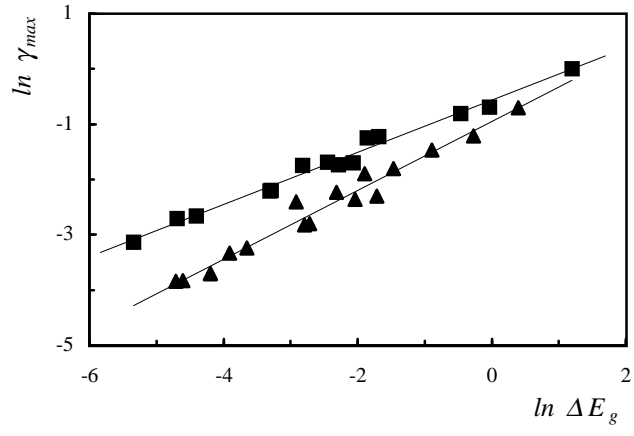


(b)

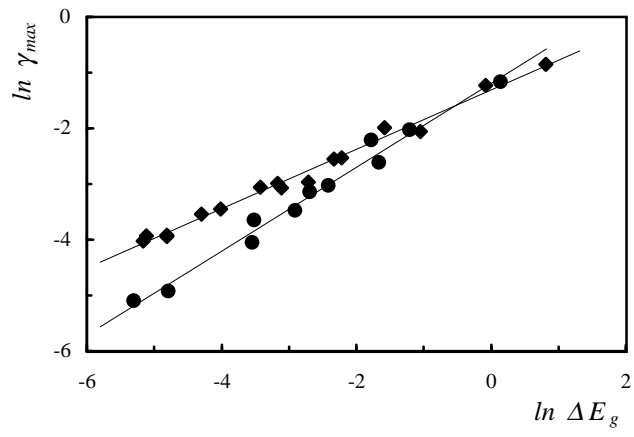


(c)

FIG. 3



(a)



(b)

FIG. 4

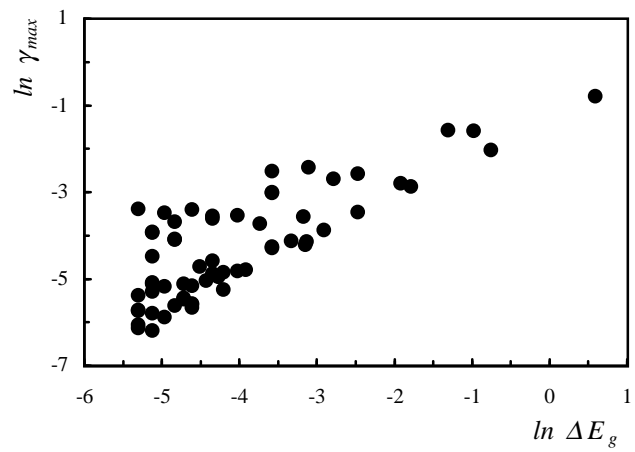
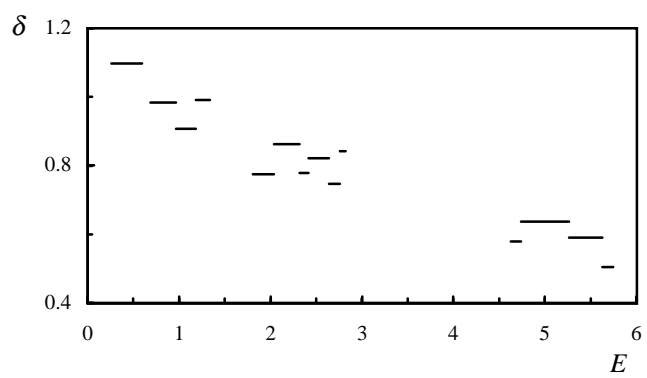
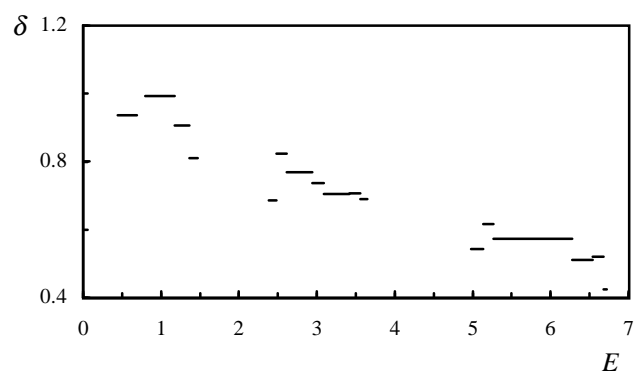


FIG. 5



(a)



(b)

FIG. 6

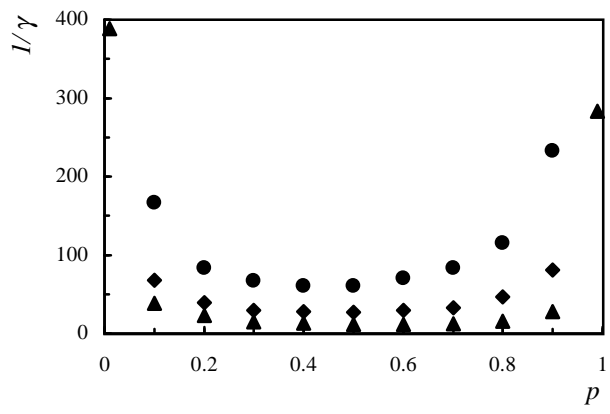
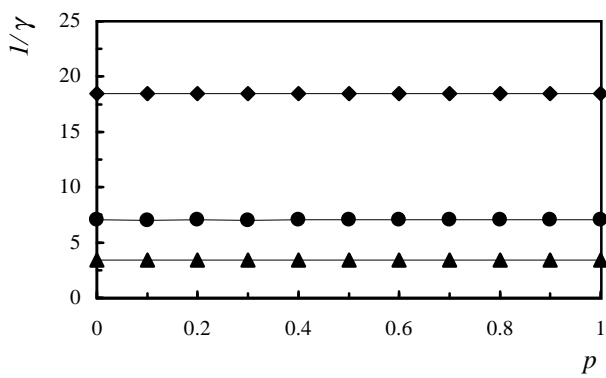
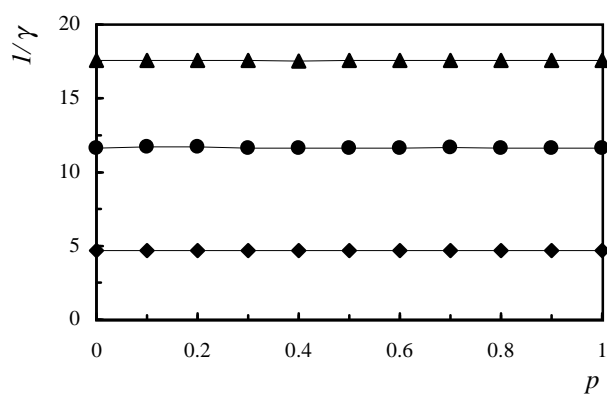


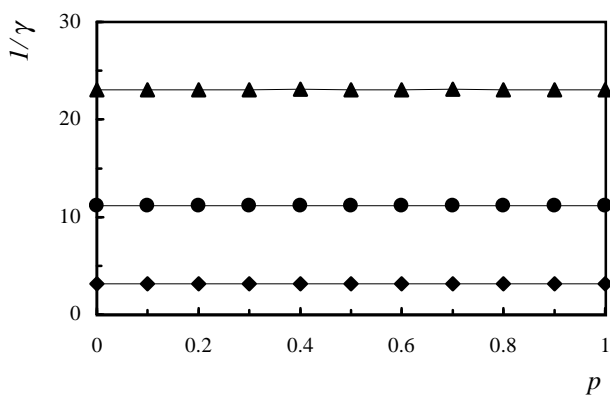
FIG. 7



(a)



(b)



(c)

FIG. 8